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Welcome to STN International! Enter x:x

LOGINID:ssspta1626gms

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

```
* * * * *
                     Welcome to STN International
NEWS
                 Web Page URLs for STN Seminar Schedule - N. America
NEWS
                 "Ask CAS" for self-help around the clock
      2
NEWS
         SEP 09
                 CA/CAplus records now contain indexing from 1907 to the
                 present
         DEC 08
                 INPADOC: Legal Status data reloaded
NEWS
         SEP 29
NEWS
      5
                 DISSABS now available on STN
         OCT 10
NEWS
                 PCTFULL: Two new display fields added
      6
         OCT 21
                 BIOSIS file reloaded and enhanced
NEWS
      7
NEWS
         OCT 28
                 BIOSIS file segment of TOXCENTER reloaded and enhanced
      8
         NOV 24
                 MSDS-CCOHS file reloaded
NEWS
     9
NEWS 10
         DEC 08
                 CABA reloaded with left truncation
NEWS 11
         DEC 08
                 IMS file names changed
                 Experimental property data collected by CAS now available
NEWS 12
         DEC 09
                 in REGISTRY
NEWS 13
         DEC 09
                 STN Entry Date available for display in REGISTRY and CA/CAplus
NEWS 14
         DEC 17
                 DGENE: Two new display fields added
NEWS 15
         DEC 18
                 BIOTECHNO no longer updated
NEWS 16
         DEC 19
                 CROPU no longer updated; subscriber discount no longer
                 available
NEWS 17
         DEC 22
                 Additional INPI reactions and pre-1907 documents added to CAS
NEWS 18
         DEC 22
                 IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields
NEWS 19
         DEC 22
                 ABI-INFORM now available on STN
NEWS 20
         JAN 27
                 Source of Registration (SR) information in REGISTRY updated
                 and searchable
         JAN 27
NEWS 21
                 A new search aid, the Company Name Thesaurus, available in
                 CA/CAplus
NEWS 22
         FEB 05
                 German (DE) application and patent publication number format
                 changes
NEWS EXPRESS
              DECEMBER 28 CURRENT WINDOWS VERSION IS V7.00, CURRENT
              MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
              AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
NEWS HOURS
              STN Operating Hours Plus Help Desk Availability
              General Internet Information
NEWS INTER
              Welcome Banner and News Items
NEWS LOGIN
NEWS PHONE
              Direct Dial and Telecommunication Network Access to STN
NEWS WWW
              CAS World Wide Web Site (general information)
```

Enter NEWS followed by the item number or name to see news on that specific topic.

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02/26/2004

Page 2 06:57 <golam shameem>

research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 06:52:23 ON 26 FEB 2004

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File ...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

### => FILE REGISTRY

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 06:52:38 ON 26 FEB 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 24 FEB 2004 HIGHEST RN 654050-72-3 DICTIONARY FILE UPDATES: 24 FEB 2004 HIGHEST RN 654050-72-3

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

Uploading C:\Program Files\Stnexp\Queries\09677021.str

# 02/26/2004

chain nodes :

10 11 12 19 20 21 22 23 24 25

ring nodes :

1 2 3 4 5 6 7 8 9 13 14 15 16 17 18

chain bonds :

 $6 - 10 \quad 10 - 11 \quad 11 - 12 \quad 12 - 16 \quad 12 - 24 \quad 12 - 25 \quad 13 - 19 \quad 19 - 20 \quad 20 - 21 \quad 21 - 22 \quad 21 - 23$ 

ring bonds :

 $1-2 \quad 1-7 \quad 2-3 \quad 3-4 \quad 4-8 \quad 5-6 \quad 5-9 \quad 6-7 \quad 7-8 \quad 8-9 \quad 13-14 \quad 13-18 \quad 14-15 \quad 15-16 \quad 16-17$ 

17-18

exact/norm bonds :

5-6 6-7 6-10 11-12 12-16 12-24 12-25

exact bonds :

5-9 8-9 10-11 13-19 19-20 20-21

normalized bonds :

 $1-2 \quad 1-7 \quad 2-3 \quad 3-4 \quad 4-8 \quad 7-8 \quad 13-14 \quad 13-18 \quad 14-15 \quad 15-16 \quad 16-17 \quad 17-18 \quad 21-22$ 

isolated ring systems :

containing 1 : 13 :

### Match level :

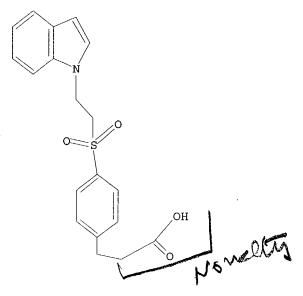
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS

#### L1STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 06:52:53 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED

2 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

2 TO 124

PROJECTED ANSWERS:

0 TO 124

L2

0 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 06:53:00 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 61 TO ITERATE

100.0% PROCESSED

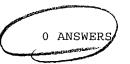
61 ITERATIONS

SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

=>

Uploading C:\Program Files\Stnexp\Queries\09677021a.str



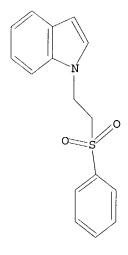
chain nodes : 10 11 12 19 20 ring nodes : 1 2 3 4 5 6 7 8 9 13 14 15 16 17 18 chain bonds : 6-10 10-11 11-12 12-16 12-19 12-20 ring bonds : 1-2 1-7 2-3 3-4 4-8 5-6 5-9 6-7 7-8 8-9 13-14 13-18 14-15 15-16 16-17 17-18 exact/norm bonds : 5-6 6-7 6-10 11-12 12-16 12-19 12-20 exact bonds : 5-9 8-9 10-11 normalized bonds : 1-2 1-7 2-3 3-4 4-8 7-8 13-14 13-18 14-15 15-16 16-17 17-18 isolated ring systems : containing 1 : 13 :

# Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS

## L4 STRUCTURE UPLOADED

=> d 14 L4 HAS NO ANSWERS L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 14

SAMPLE SEARCH INITIATED 06:54:14 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -10 TO ITERATE

100.0% PROCESSED

10 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH

\*\*COMPLETE\*\*

PROJECTED ITERATIONS:

11 TO 389

PROJECTED ANSWERS:

0 TO

 $L_5$ 

0 SEA SSS SAM L4

=> s 14 sss full

FULL SEARCH INITIATED 06:54:22 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 186 TO ITERATE

100.0% PROCESSED

186 ITERATIONS

SEARCH TIME: 00.00.01

16 SEA SSS FUL L4

L6

=> FIL CAPLUS

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY 311.26 SESSION 311.47

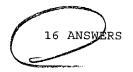
FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 06:54:33 ON 26 FEB 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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FILE COVERS 1907 - 26 Feb 2004 VOL 140 ISS 9 FILE LAST UPDATED: 25 Feb 2004 (20040225/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 16 1.7

SOURCE:

=> d 17 ibib abs hitstr tot

ANSWER 1 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:713297 CAPLUS

DOCUMENT NUMBER: 138:4442

TITLE:

Synthesis of the diketopiperazine dipodazine AUTHOR(S):

Johnson, Ann-Louise; Janosik, Tomasz; Bergman, Jan

CORPORATE SOURCE: Unit for Oranic Chem., Dept. of Biosciences, Karolinska Inst., Huddinge, SE-141 57, Swed.

ARKIVOC (Gainesville, FL, United States) [online

computer file] (2002), (8), 57-61 CODEN: AGFUAR

URL: http://www.arkat-usa.org/ark/journal/2002/Padwa/A

P-504H/AP-504H.pdf

PUBLISHER: Arkat USA Inc.

Journal; (online computer file) DOCUMENT TYPE:

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:4442

GT

Ι

The diketopiperazine derivative dipodazine (I), isolated from Penicillium AΒ dipodomyis, has been synthesized via a stereoselective aldol condensation from N-protected indole-3-carboxaldehyde and 1,4-diacetyl-2,5piperazinedione (II) in the presence of cesium carbonate.

IT 477251-70-0P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of the diketopiperazine dipodazine)

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02/26/2004

RN 477251-70-0 CAPLUS

CN 1H-Indole-3-carboxaldehyde, 1-[2-(phenylsulfonyl)ethyl]- (9CI) (CA INDEX NAME)

CHO
$$CH_2-CH_2-S-Ph$$

$$CH_2-CH_2-S-Ph$$

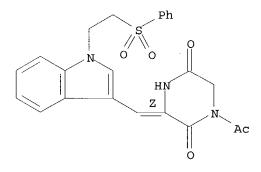
IT 477251-71-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of the diketopiperazine dipodazine)

RN 477251-71-1 CAPLUS

CN 2,5-Piperazinedione, 1-acetyl-3-[[1-[2-(phenylsulfonyl)ethyl]-1H-indol-3-yl]methylene]-, (3Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT:

THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2002:517335 CAPLUS

DOCUMENT NUMBER:

138:73142

TITLE:

N-H Insertion reactions of rhodium carbenoids. Part 3.

The development of a modified Bischler indole synthesis and a new protecting-group strategy for

indoles

AUTHOR(S):

Bashford, Katherine E.; Cooper, Anthony L.; Kane,

Peter D.; Moody, Christopher J.; Muthusamy,

Sendogagounder; Swann, Elizabeth

CORPORATE SOURCE:

School of Chemistry, University of Exeter, Exeter, EX4

4QD, UK

SOURCE:

Journal of the Chemical Society, Perkin Transactions 1

(2002), (14), 1672-1687

CODEN: JCSPCE; ISSN: 1472-7781 Royal Society of Chemistry

DOCUMENT TYPE:

PUBLISHER:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 138:73142

AB A modified version of the Bischler indole synthesis has been developed in which the key step is the N-H insertion reaction of rhodium carbene intermediates derived from  $\alpha\text{-diazo-}\beta\text{-keto}$  esters with anilines. Thus N-methylanilines react with diazo keto esters in the presence of dirhodium(II) acetate to give (N-arylamino) ketones, cyclization of which using boron trifluoride-Et acetate or acidic ion exchange resin gives indoles. In order to extend this method to the synthesis of N-unsubstituted indoles, a new protecting group strategy for indoles was developed. In this, anilines are reacted with  $\alpha,\beta\text{-unsatd}.$  esters or sulfones to give the conjugate addition products, cyclization of which gives N-protected indoles. The N-(2-ethoxycarbonylethyl)- and N-(2-sulfonylethyl)- protecting groups are readily removed from these indoles by treatment with base.

IT 413608-65-8P 413608-66-9P 413608-69-2P 413608-72-7P 480996-95-0P 480996-96-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(a modified Bischler indole synthesis and a new protecting-group strategy for indoles)

RN 413608-65-8 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3,5-dimethyl-1-[2-(phenylsulfonyl)ethyl]-,
 methyl ester (9CI) (CA INDEX NAME)

RN 413608-66-9 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-ethyl-5-methyl-1-[2-(phenylsulfonyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Et} & \text{O} \\ \text{C-OMe} \\ \\ \text{CH}_2\text{-CH}_2\text{-S-Ph} \\ \\ \text{O} \\ \end{array}$$

RN 413608-69-2 CAPLUS

CN 1H-Indole-2-carboxylic acid, 7-methoxy-3-methyl-1-[2-(phenylsulfonyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ \text{C}-\text{OMe} \\ \\ \text{OMe} & \text{CH}_2-\text{CH}_2-\text{S-Ph} \\ \\ \text{O} & \text{O} \\ \end{array}$$

RN 413608-72-7 CAPLUS

CN 1H-Indole-2-carboxylic acid, 6-methoxy-3-methyl-1-[2-(phenylsulfonyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ \text{C} & \text{OMe} \\ \\ \text{CH}_2 - \text{CH}_2 - \text{S} - \text{Ph} \\ \\ \text{O} \\ \end{array}$$

RN 480996-95-0 CAPLUS

CN 1H-Indole, 5-methoxy-1-[2-(phenylsulfonyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO} & & & \text{O} \\ & & & \text{O} \\ \text{CH}_2\text{--}\text{CH}_2\text{--}\text{S}\text{--}\text{Ph} \\ & & \text{O} \\ & & \text{O} \end{array}$$

RN 480996-96-1 CAPLUS

CN 1H-Indole-2-carboxylic acid, 1-[2-(phenylsulfonyl)ethyl]-, ethyl ester (9CI) (CA INDEX NAME)

IT 413608-67-0P 413608-68-1P 413608-70-5P

413608-71-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

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02/26/2004

(a modified Bischler indole synthesis and a new protecting-group strategy for indoles)

RN 413608-67-0 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-methoxy-3-methyl-1-[2-(phenylsulfonyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ \hline \\ \text{C}-\text{OMe} \\ \hline \\ \text{CH}_2-\text{CH}_2-\text{S}-\text{Ph} \\ \hline \\ \text{O} \\ \end{array}$$

RN 413608-68-1 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3,7-dimethyl-1-[2-(phenylsulfonyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ \hline & \text{C-OMe} \\ \hline & \text{N} & \text{O} \\ \hline & \text{CH}_2\text{-CH}_2\text{-S-Ph} \\ \hline & \text{O} \\ \hline & \text{O} \\ \hline & \text{O} \\ \hline & \text{O} \\ \hline \end{array}$$

RN 413608-70-5 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-bromo-3-methyl-1-[2-(phenylsulfonyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Br 
$$C-OMe$$
  $CH_2-CH_2-S-Ph$ 

RN 413608-71-6 CAPLUS

CN 1H-Indole-2-carboxylic acid, 4-methoxy-3-methyl-1-[2-(phenylsulfonyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2002:487554 CAPLUS

DOCUMENT NUMBER:

137:47115

TITLE:

New process for the preparation of the anti-migraine drug,

eletriptan

INVENTOR(S):

Ogilvie, Ronald James

PATENT ASSIGNEE(S):

Pfizer Limited, UK; Pfizer Inc.

SOURCE:

PCT Int. Appl., 17 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO	O. DATE	
WO 20020500	63 A1	20020627	WO 2001-IB233	B 20011206	
				BY, BZ, CA, CH, CN,	
				FI, GB, GD, GE, GH,	
				KR, KZ, LC, LK, LR,	
				MZ, NO, NZ, OM, PH,	
PL,	PT, RO, RU	J, SD, SE,	SG, SI, SK, SL, TJ,	TM, TR, TT, TZ, UA,	
UG,	US, UZ, VN	I, YU, ZA,	ZW, AM, AZ, BY, KG,	KZ, MD, RU, TJ, TM	
RW: GH,	GM, KE, LS	S, MW, MZ,	SD, SL, SZ, TZ, UG,	ZM, ZW, AT, BE, CH,	
				MC, NL, PT, SE, TR,	
			GA, GN, GQ, GW, ML,		
US 20031667	04 A1	20030904	US 2001-54727	20011113	
			AU 2002-18440		
			BR 2001-16324		
			EP 2001-271106		
				LU, NL, SE, MC, PT,	
			MK, CY, AL, TR		
PRIORITY APPLN. INFO.: GB 2000-31094 A 20001220					
			US 2001-260752P	P 20010110	
			WO 2001-IB2338	W 20011206	
OTHER SOURCE(S):	CA	ASREACT 137	:47115		

# \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The present invention is concerned with an improved process for the preparation of the anti-migraine drug, (R)-5-(2-benzenesulfonylethyl)-3-(N-

GI

methylpyrrolidin-2-ylmethyl)-1H-indole (eletriptan) (I; R = H), availablecom. as the hydrobromide salt, and with an intermediate and dimer-free products (e.g. II) obtained thereby. This process comprises coupling of Ph vinyl sulfone with 5-bromoindole derivative (III) in the presence of a palladium catalyst, a triarylphosphine, and a base, catalytic hydrogenation of the resulting 5-(2-phenylsulfonylvinyl)indole intermediate (IV) using hydrogen or hydrogen source in the presence of a suitable catalyst such as palladium on carbon, Raney nickel, platinum, rhodium, or ruthenium, and hydrolysis of the resulting precursor, i.e. N-acetyleletriptan I (R = Ac).

IT438226-83-6P

> RL: BYP (Byproduct); PREP (Preparation) (preparation of anti-migraine drug, eletriptan, by catalytic hydrogenation of (R)-1-acetyl-5-(2-benzenesulfonylethenyl)-3-(N-methylpyrrolidin-2ylmethyl)-1H-indole in presence of palladium on carbon followed by hydrolysis)

RN 438226-83-6 CAPLUS

CN1H-Indole, 3-[[(2R)-1-methyl-2-pyrrolidinyl]methyl]-1-[1-[3-[[(2R)-1methyl-2-pyrrolidinyl]methyl]-1H-indol-5-yl]-2-(phenylsulfonyl)ethyl]-5-[(1E)-2-(phenylsulfonyl)ethenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 4 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN L7

3

ACCESSION NUMBER: 2001:905624 CAPLUS

DOCUMENT NUMBER: 136:325387

A new protecting-group strategy for indoles TITLE:

AUTHOR(S): Bashford, Katherine E.; Cooper, Anthony L.; Kane,

Peter D.; Moody, Christopher J. CORPORATE SOURCE:

University of Exeter, School of Chemistry, Exeter, EX4

4QD, UK

SOURCE: Tetrahedron Letters (2001), Volume Date 2002, 43(1), 135-137

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE:

English

OTHER SOURCE(S): CASREACT 136:325387

The 2-phenylsulfonylethyl group is a useful alkyl protecting group for nitrogen during indole synthesis; it is readily removed from the indole Page 14 06:57 <golam shameem>

02/26/2004

nitrogen under basic conditions.

IT 413608-65-8P 413608-66-9P 413608-69-2P

413608-72-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(the 2-phenylsulfonylethyl protective group for nitrogen in indole synthesis)

RN 413608-65-8 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3,5-dimethyl-1-[2-(phenylsulfonyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ \text{Me} & \text{C-OMe} \\ \\ \text{CH}_2\text{-CH}_2\text{-S-Ph} \\ \\ \text{O} \\ \end{array}$$

RN 413608-66-9 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3-ethyl-5-methyl-1-[2-(phenylsulfonyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 413608-69-2 CAPLUS

CN 1H-Indole-2-carboxylic acid, 7-methoxy-3-methyl-1-[2-(phenylsulfonyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ & \text{C-OMe} \\ \\ \text{OMe} & \text{CH}_2\text{-}\text{CH}_2\text{--}\text{S-Ph} \\ \\ & \text{O} \end{array}$$

RN 413608-72-7 CAPLUS

CN 1H-Indole-2-carboxylic acid, 6-methoxy-3-methyl-1-[2-(phenylsulfonyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ \text{C}-\text{OMe} \\ \\ \text{CH}_2-\text{CH}_2-\text{S}-\text{Ph} \\ \\ \text{O} \\ \end{array}$$

TT 413608-67-0P 413608-68-1P 413608-70-5P 413608-71-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (the 2-phenylsulfonylethyl protective group for nitrogen in indole synthesis)

RN 413608-67-0 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-methoxy-3-methyl-1-[2-(phenylsulfonyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ \hline & \text{C-OMe} \\ \hline & \text{N} & \text{O} \\ \hline & \text{CH}_2\text{-CH}_2\text{-}\text{S-Ph} \\ \hline & \text{O} \\ \hline & \text{O} \\ \hline \end{array}$$

RN 413608-68-1 CAPLUS

CN 1H-Indole-2-carboxylic acid, 3,7-dimethyl-1-[2-(phenylsulfonyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} \\ \text{C-OMe} \\ \\ \text{N} & \text{O} \\ \\ \text{CH}_2\text{--}\text{CH}_2\text{--}\text{S--Ph} \\ \\ \text{Me} & \text{O} \\ \end{array}$$

RN 413608-70-5 CAPLUS

CN 1H-Indole-2-carboxylic acid, 5-bromo-3-methyl-1-[2-(phenylsulfonyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

Br 
$$C-OMe$$
  $C+CH_2-CH_2-S-Ph$   $C+CH_2-CH_2-S-Ph$ 

RN413608-71-6 CAPLUS

> 1H-Indole-2-carboxylic acid, 4-methoxy-3-methyl-1-[2-(phenylsulfonyl)ethyl]-, methyl ester (9CI) (CA INDEX NAME)

OMe Me 
$$C-OMe$$

$$C-OMe$$

$$CH_2-CH_2-S-Ph$$

REFERENCE COUNT:

10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1991:583011 CAPLUS

DOCUMENT NUMBER:

115:183011

TITLE:

CN

Sulfenylation of some pyrroles and indoles

AUTHOR(S):

Gilow, Helmuth M.; Brown, Christopher S.; Copeland,

John N.; Kelly, Keith E.

CORPORATE SOURCE: SOURCE:

Chem. Dep., Rhodes Coll., Memphis, TN, 38112, USA Journal of Heterocyclic Chemistry (1991), 28(4),

1025-34

CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE:

Journal

LANGUAGE: English

Methylsulfenylation of 1-substituted pyrroles and indoles was observed using 1-(methylthio)morpholine and an acid catalyst or with methylsulfenyl chloride and excess pyridine. 1-Substituents which are activating or weakly deactivating towards electrophilic substitution such as alkyl, 2-cyanoethyl, dimethylamino, trialkylsilyl, 2-chloroethyl and 2-phenylsulfonylethyl were used. The 2-chloroethyl and 2-phenylsulfonylethyl groups which can be removed with a strong base can be used to obtain 1H-methylthiopyrroles and indoles. 1-Phenylsulfonyl and 1-acetyl substituents are too strongly deactivating for these sulfenylations to be successful. Mono- and disubstituted pyrroles and monosubstituted indoles can be isolated from these reactions, however, because the methylthio group is activating towards electrophilic substitution the main advantage of these reactions is the synthesis of tri- and tetrasubstituted pyrroles and disubstituted indoles. 1-Methyl-2,3,4,5-tetrakis (methylthio) pyrrole and 1-methyl-2,3bis (methylthio) indole are oxidized to the corresponding 3,4-disulfoxide and 3-sulfoxide and with excess oxidizing agent to the tetrasulfone and

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02/26/2004

disulfone, resp.

IT136506-30-4P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and deblocking of)

RN136506-30-4 CAPLUS

CN 1H-Indole, 1-[2-(phenylsulfonyl)ethyl]-2,3-bis(phenylthio)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CH_2-CH_2-S-Ph \\ & \parallel \\ N & SPh \end{array}$$

136506-29-1P, 1-(2-Phenylsulfonylethyl) indole IT

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and sulfenylation of)

RN 136506-29-1 CAPLUS

CN1H-Indole, 1-[2-(phenylsulfonyl)ethyl]- (9CI) (CA INDEX NAME)

ANSWER 6 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1982:199522 CAPLUS

DOCUMENT NUMBER:

96:199522

TITLE:

Acylindole derivatives

PATENT ASSIGNEE(S):

Teijin Ltd., Japan

SOURCE:

Jpn. Kokai Tokkyo Koho, 22 pp. CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE		APPLICATION NO.	DATE
JP 57004971	A2	19820111		JP 1980-78305	19800612
PRIORITY APPLN. INFO.	:		JP	1980-78305	19800612
GI					

Twenty-one acylindole derivs. I [R = (un) substituted Ph; R1 = H, alkyl; R2 = alkyl; R3 = H, OH, halo, alkyl, alkoxy; R4 = S(0)m R5; F5 = H, alkyl, (un) substituted Ph, heterocycle; n = 1-10; m = 0-2] were prepared I had platelet aggregation inhibitory activity (data given). Thus, a mixture of 586 mg I (R = Ph, R1 = R2 = Me, R3 = H, R4 = OH n = 1), 732 mg EtSSEt, and 1.5 mL Bu3P in pyridine was stirred 16 h at room temperature and 8 h at 50° to give 77% I (R = Ph, R1 = R2 = Me, R3 = H, R4 = SEt, n = 1).

IT 77993-46-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and platelet aggregation inhibitor activity of)

RN 77993-46-5 CAPLUS

CN Methanone, [2-methyl-1-[1-methyl-2-(phenylsulfonyl)ethyl]-1H-indol-3-yl]phenyl- (9CI) (CA INDEX NAME)

ANSWER 7 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

Ι

ACCESSION NUMBER: 1981:424812 CAPLUS

DOCUMENT NUMBER: 95:24812

TITLE: Acylated indole derivatives

INVENTOR(S): Oba, Takeo; Tanaka, Toshio; Okamura, Noriaki;

Watanabe, Kenzo; Bannai, Kiyoshi; Ohtsu, Akira;

Naruchi, Tatsuyuki; Kurozumi, Seizi; Toru, Takeshi

PATENT ASSIGNEE(S): Teijin Ltd., Japan

SOURCE: Eur. Pat. Appl., 145 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

EP 22634 A1 19810121 EP 1980-302180 19800627

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EP 22634	B1	19830406			
R: DE, FR, G	B, IT	, SE			
JP 56007762	A2	19810127		JP 1979-80802	19790628
JP 62033225	B4	19870720			
JP 56039068	A2	19810414		JP 1979-112755	19790905
JP 56051452	A2	19810509		JP 1979-126725	19791003
JP 62041499	B4	19870903			
JP 56063960	A2	19810530		JP 1979-138644	19791029
JP 62041500	B4	19870903			
JP 56108765	A2	19810828		JP 1980-8354	19800129
JP 62041590	B4	19870903			
PRIORITY APPLN. INFO.:			JP	1979-80802	19790628
			JP	1979-112755	19790905
			JΡ	1979-126725	19791003
			JΡ	1979-138644	19791029
			JΡ	1980-8354	19800129
OTHER SOURCE(S):	CAS	SREACT 95:248	312		

AB Indoles I (R = optionally substituted Ph, thienyl; R1, R3 = H, alkyl; R2 = alkyl; R4 = H, alkyl, acyl, optionally substituted Ph, heterocyclic; R5 = H, OH, halogen, alkyl, alkoxy; X = bond, O, S, S0, S02; n = 0-10) were prepared Thus 2-acetonylcyclohexanone was condensed with H2NCHMeCO2Et.HCl to give II (R6 = CHMeCO2Et) which was reduced to the alc. and esterified to II (R6 = CHMeOAc). The latter compound was benzoylated with Bz20 and HI, followed by aromatization, to give I (R = Ph, R1 = R2 = Me, R4 = Ac, R5 = H, X = O, n = 0)(III). III had a blood platelet aggregation-inhibiting ED50 of 0.075  $\mu/mL$ .

IT 77993-46-5P

GΙ

RN 77993-46-5 CAPLUS

CN Methanone, [2-methyl-1-[1-methyl-2-(phenylsulfonyl)ethyl]-1H-indol-3-yl]phenyl- (9CI) (CA INDEX NAME)

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02/26/2004

-4.85

-4.85

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